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MASSACHUSETTS INSTITUTE OF TECHNOLOGY

LINCOLN LABORATORY

PRACTICAL ASPECTS OF GAUSSIAN INTEGRATION

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ABSTRACT

A method for accurate numerical integration is proposed and illustrated by a variety of examples. The method depends on an ability to efficiently evaluate the weights and abscissas of Gaussian quadrature formulas, and software to achieve this purpose is also presented.

CONTENTS

I. INTRODUCTION

A considerable number of problems of physical and engineering interest require as part of their solution the accurate evaluation of definite integrals of the form

$$\int_R f(x)dx, \qquad [*]$$

where R is a closed region of one or more dimensions. Typical cases have R = a compact or infinite interval in one dimension, and R = a rectangular or spherical solid in higher dimensions. In applications, the integral [*] may yield percentage points of a probability distribution, the autocorrelation of a signal, a one or two dimensional convolution of a signal with a filter response function, the intensity of graybody radiation emitted into a particular waveband (Planck integral), certain thermodynamic lattice sums, etc.

Usually it is desired that the computed value of [*] be accurate to so many digits (prescribed relative error) or to so many decimal digits (prescribed absolute error). The only way that a user can be <u>certain</u> that this requirement is satisfied is to have available an error formula for the integration rule being employed, and to verify that the integrand and the order of the rule are such that the error term is sufficiently small. (In making this last statement we are assuming negligible roundoff error.) Now typically the classical error term (for integration over intervals) involves a small coefficient multiplied by a high order derivative evaluated at an unknown point in the interval of integration. Hence in practice the maximum modulus of this derivative must be computed or at least bounded. And in practice this task is usually impossible, due to the complexity of the intergrand.

One way out of this difficulty (for the case where R is a compact interval) is available when the integrand f extends to an analytic function on some neighborhood of R. Complex variable methods (related to the Cauchy integral formula) then often permit bounds on the error in terms only of the values of f, and not of its derivatives. Furthermore, the error term will tend exponentially to zero, as the order of the integration rule increases. Unfortunately, it is not always the case that our integrand is analytic.

This note will present a procedure for resolving the problem of fast accurate quadrature for integrands which are reasonably smooth but not necessarily analytic. In the absence of smoothness (i.e., if there are discontinuities in the first derivative, or in one of the first partial derivatives, if the integrand is a function of several variables), our method will not have favorable convergence properties, and should not be employed. In the case of integration over a compact interval, one would then be better advised to utilize a trapezoidal-type rule, such as (adaptive) Romberg integration [1, § 6.3]. Software for such a procedure is available in the International Mathematical and Statistical Library (IMSL) under the title DCADRE.

In brief, our method is based on observation of the convergence of a sequence of Gauss-type quadratures with appropriate weight function. For this to be practical it is necessary to have available a fast procedure for generating the abscissas and coefficients of a Gaussian formula of a given order. Such a procudure is given below; it is based on suggestions of Wilf [2] and Golub-Welsch [3] to convert this problem to an eigenanalysis of a certain (symmetric) matrix.

The original motivation for this work came from the (two-dimensional) problem of accurately computing the overall output of an optical detector [4, § 6.2.2.1.1]. This output is the convolution of the detector response function and the irradiance function H. In the important special case of a rectangular detector this convolution reduces to the integration of H over the (rectangular) detector surface. Our method, described below, was proposed as an alternative to the use of fast Fourier transform techniques, with their arbitrary sampling decisions and apparent lack of suitable error theory.

II. REVIEW OF GAUSSIAN QUADRATURE THEORY

This section contains a brief exposition of convergence and error analysis for Gaussian integration formulas. No attempt has been made to write a small text on the subject! For further background the sources [1, 5, 6, 7] may be consulted. In general the recent monograph [1] is an excellent source of information about all aspects of the quadrature problem.

2.1 Basic Theory

Let I be an interval of real numbers and let ω be a weight function on I, that is, $\omega(x) \geq 0$ and $\int_I x^n \omega(x)dx$ is finite for $n = 0,1,2,\cdots$. Then there exists a sequence $\{p_n(x): n = 0,1,2, \ldots\}$ of polynomials of degree n with are orthonormal on I with respect to ω, in the sense that

$$\int_I p_m(x)\ p_n(x)\ \omega(x)dx = \delta_{mn}\ , \tag{2.1}$$

for all m,n, = $0,1,2,\cdots$. These p_n are unique up to a sign, and we shall adjust this sign so that the coefficient k_n of x^n in p_n is positive. The p_n can be computed either by applying the Gram-Schmidt procedure to the monomials $\{x^n\}$ or by use of a recurrence relation

$$p_n(x) = (a_n x + b_n)\ p_{n-1}(x) - c_n\ p_{n-2}(x), \tag{2.2}$$

where $a_n, c_n \neq 0$, $p_{-1}(x) = 0$, $p_0(x) = (\int_I \omega(x)dx)^{-\frac{1}{2}}$. This recurrence will be very important to us below. Let us now just note one special relation between the coefficients a_n and c_n that follows from the normality of the p_n. Namely, by multiplying both sides of (2.2) by $p_n\omega$ and by $p_{n-2}\omega$ and integrating over I, we obtain

$$1 = a_{n-1} \int_I x p_{n-1}(x)\ p_{n-2}(x)\omega(x)dx,$$

$$0 = a_n \int_I x p_{n-1}(x)\ p_{n-2}(x)\omega(x)dx - c_n,$$

whence

$$c_n = a_n/a_{n-1} \tag{2.3}$$

Now consider the n x n tridiagonal symmetric (Jacobi) matrix

$$A = \begin{bmatrix} -b_1/a_1 & c_2/a_2 & 0 & 0 & \cdot\cdot & 0 \\ c_2/a_2 & -b_2/a_2 & c_3/a_3 & 0 & \cdot\cdot & 0 \\ 0 & c_3/a_3 & -b_3/a_3 & c_4/a_4 & \cdot\cdot & 0 \\ 0 & 0 & \cdots & & c_n/a_n & -b_n/a_n \end{bmatrix}$$

Using (2.3) the reccurrence relation (2.2) can be rewritten in the matrix-vector format

$$AP(x) = xP(x) + \frac{c_{n+1}}{a_{n+1}} p_n(x) \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}, \tag{2.4}$$

where $P(x) = (p_o(x), p_1(x), \ldots, p_{n-1}(x))^T$. From (2.4) we conclude that a real number x_o is a root of p_n exactly when it is an eigenvalue of A. [2,3].

The reason for our interest in the roots of p_n is of course that they comprise the abscissas of the corresponding Gauss quadrature rules. The n^{th} Gauss quadrature formula is a (positive) linear functional whose value at a continuous function f is

$$G_n(f;\omega) = \sum_{k=1}^{n} \omega_k^{(n)} f(x_k^{(n)}), \tag{2.5}$$

where

$$0 < \omega_k^{(n)} = -\frac{k_{n+1}}{k_n} (P_{n+1}(x_k^{(n)})\ P_n'(x_k^{(n)}))^{-1}, \qquad 1 \leq k \leq n.$$

With this choice of weights $\{\omega_k^{(n)}\}$ and abscissas $\{x_k^{(n)}\}$ it is well known [1] (see also § 3.2 below) that

$$\int_a^b f(x)\omega(x)dx = G_n(f;\omega) + \frac{f^{(2n)}(\xi)}{(2n)!\, k_n^2}, \quad a<\xi<b \qquad (2.6)$$

provided that a,b are finite and f has 2n continuous derivatives on [a,b]. A particular import of (2.6) is that the Gauss rule of order n exactly integrates every polynomial of degree $\leq 2n - 1$. This is the famous optimality property of Gauss rules: they are exact for polynomials of as large a degree as is possible with a formula of the type (2.5) (there are only 2n free parameters in (2.5)).

2.2 Error Analysis

Let $E_n(f)$ denote the error in uniform approximation on [a,b] to the continuous function f by polynomials of degree $\leq n$. If p is such a polynomial then the error in n^{th} order Gauss quadrature, $EG_n(f;\omega)$, satisfies

$$|EG_n(f;\omega)| = \left|\int_a^b f(x)\omega(x)dx - G_n(f;\omega)\right|$$

$$\leq \left|\int_a^b (f(x)-p(x))\omega(x)dx\right| + |G_n(f-p;\omega)|$$

$$\leq \left(\int_a^b \omega(x)dx + \sum_{k=1}^{n} \omega_k^{(n)}\right) \max_{a\leq x\leq b} |f(x)-p(x)|$$

$$= 2\int_a^b \omega(x)dx \quad ||f-p||_\infty . \tag{2.7}$$

This being true for all polynomials of degree $\leq 2n-1$, we conclude that

$$|EG_n(f;\omega)| \leq 2\int_a^b \omega(x)dx \cdot E_{2n-1}(f) \tag{2.8}$$

The advantage of (2.8) over (2.6) is first, that there is no derivative assumption made about f, and second, that upper bounds for the error can always be obtained by use of (2.7). Of course the best theoretical estimates of $E_n(f)$ depend on derivative information about f ("Jackson's theorems", [6]).

In the most favorable situation for Gaussian quadrature on a compact interval [a,b], the integrand f is (the restriction of) an analytic function on [a,b]. Then it is known ("Bernstein's theorem", [6]) that the quantities $E_n(f)$ decrease very rapidly; precisely,

$$E_n(f) \leq Kq^n,$$

for positive constants K and q, with $q < 1$. Hence, by virtue of (2.8) the Gauss quadratures of f converge at essentially a geometric rate ("r-linear convergence") to the true value of

$\int_a^b f(x)\omega(x)dx$. (There is in fact an extensive literature on error estimates for Gauss quadratures of analytic functions, giving more precise versions of this fact; see [8] for a recent contribution.)

The last two paragraphs strongly suggest that Gaussian quadrature will be most effective for integrands which exhibit polynomial behavior, and this is certainly true in a practical sense, when computation time is an issue. But, in fact, the estimate (2.8) and the Weierstrass approximation theorem show that

$$\lim_{n\to\infty} G_n(f;\omega) = \int_a^b f(x)\omega(x)dx. \tag{2.9}$$

holds true whenever f is a continous function on [a,b]. Indeed, (2.9) is valid whenever $f\omega$ is Riemann integrable on [a,b] [9].

2.3 Double Integrals

Let us now consider the problem of numerically evaluating a multiple integral over a rectangular region R = [c,d] x [a,b]. The ensuing discussion applies as well to solid rectangular regions in 3 or more dimensions, and integrals over other types of regions can frequently be reduced to integrals over rectangular ones by means of appropriate transformations of coordinates [1, § 5.4].

A standard approach to evaluation of

$$\int_a^b \int_c^d f(x,y)\omega(x)\omega(y)dx\,dy \tag{2.10}$$

is to apply one-dimensional quadrature formulas to the functions $f(x,\cdot)$ and $f(\cdot,y)$. The resulting formula is known as a product rule [1, § 5.6, 10, § 2.3] and in the case that each one-dimensional formula is $G_n(\cdot;\omega)$, we can obtain the product Gauss formula

$$G_n^{(2)}(f;\omega) = \sum_{i=1}^{n} \sum_{j=1}^{n} \omega_i^{(n)}\omega_j^{(n)} f(x_i^{(n)}, x_j^{(n)}) \tag{2.11}$$

as an approximation to (2.10). Although the theory of multivariate polynomial approximation is not as well developed as the single variable case, there is still a Weierstrass theorem. Hence, since (2.11) will integrate any polynomial $p(x,y)$ exactly provided that n is sufficiently large, we may conclude that

$$\lim_{n\to\infty} G_n^{(n)}(f;\omega) = \int_a^b \int_c^d f(x,y)\omega(x)\omega(y)dxdy, \tag{2.12}$$

for all continuous functions on R.

What about the validity of (2.12) when the integrand in (2.10) is merely Riemann integrable? The difficulty here is that this assumption need not imply that the sections $f(x,y)\omega(x)$ and

$f(x,y)\omega(y)$ be integrable on $[c,d]$ and $[a,b]$, respectively. Hence, in general there will be no reason to expect the product Gauss rule to converge. But suppose that the integral (2.10) is well enough behaved to obey the Fubini iterated integrals formula:

$$\int_a^b\int_c^d f(x,y)\omega(x)\omega(y)\,dxdy = \int_a^b \left(\int_c^d f(x,y)\omega(x)\,dx\right)\omega(y)\,dy. \quad (2.13)$$

Denoting the inner integral in (2.13) by $f(y)$, we can compute $G_n(f;\cdot)$ for a sufficiently large n; then we can approximately compute each value $f(x_k^{(n)})$ for $k = 1,\ldots,n$ by Gaussian formulas $G_m(f(\omega,x_k^{(n)}))$ for sufficiently large m. In this way we can conclude that

$$\lim_{n\to\infty}\lim_{m\to\infty}\sum_{i=1}^{n}\sum_{j=1}^{m}\omega_i\omega_j\, f(x_j^{(m)}, x_i^{(n)}) = \int_a^b\int_c^d f(x,y)\omega(x)\omega(y)\,dxdy.$$

This convergence result is clearly less satisfactory than (2.12) although it could be used in practice provided (2.13) could be verified.

2.4 Infinite Interval

Finally we consider the matter of the validity of the convergence formula (2.9) when $b = \infty$. This is not covered by the earlier analysis on account of the non-compactness of the interval $[a,\infty)$. However, it is shown in [5, § III.1] that for a class of positive quadrature rules which includes the important special case of the Gauss-Laguerre formula with weight function $\omega(x;\alpha) = x^{\alpha}e^{-x}$ $(\alpha>-1)$, convergence is obtained for every function f such the $f(\cdot)\omega(\cdot;\alpha)$ is Riemann integrable on $[a,\infty)$, and f has at most polynomial growth at ∞. The proof depends on being able to "squeeze" f between two polynomials: $p_1 \leq f \leq p_2$, such that $\int_a^{\infty}(p_2(x) - p_1(x))\omega(x;\alpha)dx$ is arbitrarily small.

III. THE PROPOSED METHOD

Armed with this theoretical underpinning of convergence theory we can in practice proceed to evaluate an integral of the form [*] (Introduction) by simply observing the behavior of a sequence of approximations $G_n(f;\omega)$: $n=1, 2, \ldots$, and terminating the process when $|G_{n+1}(f;\omega) - G_n(f;\omega)| < \varepsilon$, for some preassigned tolerance ε. There are several caveats to be mentioned here. First, this termination criterion cannot conclusively prove that $G_n(f;\omega)$ is adequately close to [*] (cf. the discussion in [1, § 6.1]). It is always possible to construct ad hoc counterexamples. Nevertheless, this does not seem to be a difficulty in practice, although it would be safer to require that the termination criterion above hold for 2 or 3 successive values of n. Second, there is the matter of choice of weight function, especially when one is not obviously present to begin with. Third, there is the need to be able to efficiently generate the weights and abscissas necessary to fully specify the value $G_n(f;\omega)$ for various values of n. Finally, this method should, as already noted, only be applied in cases where the integrand f is reasonably smooth; otherwise convergence is likely to be too slow to be useful.

The choice of weight function will be discussed in the following sections. As to the third point just raised, the key here is the use of the eigenvalue problem shown in formula (2.4). By computing the eigenvalues of the Jacobi matrix A we obtain the abscissas of the corresponding Gauss formula. Further it is known that

$$1 = \omega_k^{(n)} \; P(x_k^{(n)})^T \; P(x_k^{(n)}),$$

where P(x) was defined just after (2.4). Hence

$$Q_k^{(n)} \equiv \sqrt{\omega_k^{(n)}} \; P(x_k^{(n)})$$

is a normalized eigenvector of A corresponding to the eigenvalue $x_k^{(n)}$. By considering just the first component of $P(x_k^{(n)})$ we can conclude that

$$\omega_k^{(n)} = \int_I \omega(x)\,dx \cdot (Q_k^{(n)})_1^2.$$

In other words, the various weights $\omega_k^{(n)}$ associated with the Gauss formula $G_n(\cdot;\omega)$ can be obtained as the constant $\int_I \omega(x)dx$ times the square of the first component of a system of n orthonormal eigenvectors associated with the matrix A.

FORTRAN codes illustrating this procedure for several weight functions and numerical illustrations of the whole method will be given in the ensuing sections, along with further discussion. It is important to appreciate the ease and accuracy with which the weights and abscissas can be computed in this manner. Earlier efforts were much slower. They typically involved the use of some root finding scheme, such as Newton's method, applied directly to locate each zero of the relevant polynomial. All the usual attendant difficulties arose here, such as the need for a sufficiently accurate starting value. This was particularly a problem in trying to locate the zeros of the generalized Gauss-Laguerre polynomials (corresponding to the weight function $\omega(x;\alpha) = x^{\alpha}e^{-x}$, $\alpha > -1$, on $[0,\infty)$), as these tend to drift off to infinity as either α or n increase. See, for example, the discussion in [11].

IV. GAUSS-CHEBYSHEV QUADRATURE

We first look at the case where the weight function $\omega(x) = (1-x^2)^{-\frac{1}{2}}$ on $[-1, 1]$. Thus the resulting quadrature formula (2.5) will approximate

$$\int_{-1}^{1} \frac{f(x)dx}{\sqrt{1-x^2}} . \tag{3.1}$$

The orthonormal polynonials associated with this ω are the well-known Chebyshev polynomials:

$$p_n(x) = \sqrt{\tfrac{2}{\pi}}\, T_n(x) = \sqrt{\tfrac{2}{\pi}} \cos(n \cos^{-1}x), \quad n \geq 1$$

$$p_0(x) = \frac{1}{\sqrt{\pi}} .$$

In this case we may clearly write down the roots of p_n (= the abscissas of the corresponding Gauss formula) by inspection:

$$x_k^{(n)} = \cos\left(\frac{2k-1}{2n}\pi\right) , \qquad 1 \leq k \leq n.$$

Further, although less obvious, the associated weights $\omega_k^{(n)} = \pi/n$, $1 \leq k \leq n$, independently of k [6, v.2, ch.5]. It is interesting that this is the <u>only</u> case where this property of the weights holds true (assuming the interval is fixed as [-1, 1]; this is Posse's theorm [6, v.2, Ch.6]).

Combining all this information the general formula (2.6) here appears as

$$\int_{-1}^{1} \frac{f(x)\,dx}{\sqrt{1-x^2}} = \frac{\pi}{n} \sum_{k=1}^{n} f(\cos(\frac{2k-1}{2n}\pi)) + \frac{2\pi\ f^{(2n)}(\xi)}{4^n (2n)!}, \qquad (3.2)$$

for some $|\xi| < 1$, provided $f \varepsilon C^{2n}[-1, 1]$. This formula is remarkable because the weights and abscissas appear in closed form; the eigenanalysis of the preceding section is not needed here for their computation.

4.1 Program and Examples

Exhibit 1 gives a short FORTRAN program which enables a user to calculate an n^{th} order Gauss-Chebyshev approximation to any integral of the form

$$\int_{a}^{b} g(y)\,dy; \qquad (3.3)$$

the programs accepts a, b, and n as inputs and calculates the corresponding quadrature (after an appropriate change of variable). Because in general the integral (3.3) does not contain the weight function ω as a factor, it is introduced artifically in the FUNC-

```
C    PROGRAM TO DO ONE DIM. GAUSS-CHEBYSHEV QUADRATURE
C
      COMMON A,B
      WRITE(6,1)
1     FORMAT(1X,'ONE DIM. GAUSS-CHEBYSHEV QUADRATURE',//,
     &1X,'INPUT LOWER AND UPPER END POINTS')
      READ(5,*) A ,B
25    WRITE(6,2)
2     FORMAT(1X,'INPUT ORDER OF G-CHB. FORMULA')
      READ(5,*) N
      CALL TIMES(D1,T1,IV,IT)
      PI2 = ASIN(1.)
      QNF = 0.
      DO 5 K=1,N
      XKN = COS((2*K-1)*PI2/N)
      QNF = QNF + F(XKN)
5     CONTINUE
      QNF = QNF*(B-A)*PI2/N
      CALL TIMES(D2,T2,IV2,IT2)
      ETIM = FLOAT(IV2-IV)*.000013
      WRITE(6,10) N, QNF
10    FORMAT(/1X,'G-CHB. QUAD(F;',I3,') =  ,F12.6)
      WRITE(6,12) ETIM
12    FORMAT(/1X,'EXECUTION TIME = ',F7.3)
      WRITE(6,20)
20    FORMAT(/1X,'RESTART? INPUT 0(NO) OR 1(YES)')
      READ(5,*) NR
      IF (NR .EQ. 0) STOP
      GO TO 25
      END
C
C
      FUNCTION F(X)
      COMMON A,B
      Y = .5*(A+B+(B-A)*X)
C  ENTER INTEGRAND NEXT AS FCN. OF Y
      G = 2./(2.+SIN(10.*ACOS(-1.)*Y))
      F = G*SQRT(1.-X**2)
      RETURN
      END

R; T=0.02/0.19 14:43:34
```

Exhibit 1

TION subprogram. This feature may cause the sequence of Gauss-Chebyshev quadratures to converge more slowly than the corresponding sequence of Gauss-Legendre quadratures discussed in the next section (where the weight function $\equiv 1$), but the simplicity of formula (3.2) still is a cogent argument for its use.

Table 1 gives some sample output for an assortment of definite integrals. Since the computation was carried out in single precision IBM 370 arithmetic, only 5 significant figures are given. Observe that in all cases except the last convergence (to 5 figures) is achieved by an order 200 formula. The time column gives the execution times required to compute the last entry in each row. These times are a bit higher than necessary in most cases because of the large increases in N. That is, if we increased N more slowly, say by increments of 5 or 10, we would generally achieve convergence to 5 places sooner than shown in Table 1, with a correspondingly reduced execution time.

TABLE 1

EXAMPLES OF GAUSS-CHEBYSHEV QUADRATURE

Integral	N = 10	25	50	100	150	200	True	Time
$\int_0^1 y^{3/2}dy$	.40208	.40033	.40008	.40001	.40000	——	.40000	.011 sec.
$\int_0^3 e^{2y}dy$	230.783	201.615	201.314	201.235	201.218	201.213	201.214	.015 sec.
$\int_0^1 y\sqrt{4-y^2}dy$	.93818	.93519	.93475	.93464	.93462	——	.93462	.011 sec.
$\int_0^1 \frac{dy}{1+y^4}$	.87006	.86747	.86709	.86700	.86698	.86697	.86697	.013 sec.
$\int_0^1 \frac{2dy}{2+\sin 10\pi y}$	1.20395	1.15548	1.15492	1.15473	1.15471	1.15470	1.15470	.017 sec.
$\int_{-1}^1 (1-\lvert y\rvert)dy$	.99161	1.00263	.99967	.99991	.99995	.99997	1.0000	.012 sec.

4.2 Unilateral Error Bounds

A final remark about Gauss-Chebyshev quadrature pertains to the possibility of a one-sided error bound, in the sense that for some integrands f it may happen that either

$$G_n(f;\ \text{Chb.}) \le \int_{-1}^{1} \frac{f(x)\,dx}{\sqrt{1-x^2}}, \qquad (3.3)$$

or

$$G_n(f;\ \text{Chb.}) \ge \int_{-1}^{1} \frac{f(x)\,dx}{\sqrt{1-x^2}}, \qquad (3.4)$$

for all n. For example, inequality (3.4) is valid for the first three integrals in Table 1, and also holds for the fourth integral, provided that $n \ge 4$.

These inequalities would obviously follow from the stronger results of monotone convergence

$$G_n(f;\ \text{Chb.}) \le G_{n+1}(f;\ \text{Chb.}) \qquad (3.3\text{m})$$

or

$$G_n(f;\ \text{Chb.}) \ge G_{n+1}(f;\ \text{Chb.}), \qquad (3.4\text{m})$$

for all n (or, for all sufficiently large n). In this section we give some conditions of f sufficient to ensure one of the preceding inequalities (3.3) or (3.4).

In general, let

$$EG_n(f;\ Chb.) = \int_{-1}^{1} \frac{f(x)dx}{1-x^2} - G_n(f;\ Chb.)$$

be the error in the Gauss-Chebyshev rule. One expression for $EG_n(f;\ Chb.)$ was given in (3.2), as a special case of (2.6). For the general case of Gauss-Jacobi quadrature (where the weight function $\omega(x) = (1-x)^{\alpha}\ (1+x)^{\beta}$, $-1<\alpha, \beta, |x|\leq 1)$, we can deduce (2.6) and hence (3.2) from the Peano kernel theorem [1, p. 18] which permits us to write

$$EG_n(f;\omega) = \int_{-1}^{1} K_{\omega}^{(n)} f^{(2n)}(t)dt \tag{3.5}$$

for every $f\epsilon\ C^{2n}[-1,\ 1]$. Here $K_{\omega}^{(n)}$ is a certain "kernel" which depends on the weight fucntion ω and the order n. It is known that $K_{\omega}^{(n)}$ is of class C^{2n-2} on $[-1,\ 1]$, is positive for $|t|<1$, and in the $\alpha=\beta$ (ultraspherical) case, $K_{\omega}^{(n)}$ is an even function [12, Ch. 4].

Now consider the special integrand $f(x) = x^p$, $p=0,\ 1,\ 2,\cdots$. Applying (3.5) we have

$$EG_n(x^p;\ \omega) = p(p-1)\cdots(p-2n+1) \int_{-1}^{1} K_{\omega}^{(n)}(t)^{p-2n}dt$$

$$= \begin{cases} 2p(p-1)\cdots(p-2n+1) \displaystyle\int_0^1 K_\omega^{(n)}(t)\,t^{p-2n}dt \geq 0, & \text{if } p \text{ is even,} \\ 0 \quad , & \text{if } p \text{ is odd,} \end{cases}$$

provided that $K_\omega^{(n)}$ is an even function. These equations remain true if f is replaced by any polynomial with positive coefficients, or a limit of such polynomials. Hence, for such functions, inequality (3.3) is valid (note that this result has been demonstrated to hold for all Gauss quadrature formulas derived from ultraspherical polynomials, in particular for the Gauss-Legendre rule of the next section).

A general class of integrands for which (3.3) is valid is, for instance, the class of analytic functions f on (-1,1) with

$$f^{(p)}(0) \geq 0, \quad p = 1, 2, 3, \ldots \quad . \tag{3.6}$$

And by starting with $f(x) = -x^p$, $p = 1, 2, 3, \ldots$, and repeating the above analysis, we can obtain a class of functions for which inequality (3.4) is valid, namely, the class of analytic functions f for which (3.6) holds with the opposite inequality sign. Empirical evidence suggests that in fact the stronger inequalities (3.3m) and (3.4m) hold for these two classes of integrands respectively.

Another condition sufficient to ensure one of the estimates (3.3) or (3.4) follows immediately from the error formula (3.2). Namely, if f has derivatives of all orders on (-1, 1) and $f^{(2n)}(x) \geq 0$ (resp. ≤ 0) on (-1, 1), then inequality (3.3) (resp. (3.4)) is valid. Indeed this condition may be established for quite general weight functions, as was originally shown by Shohat; see [5, p. 92].

V. GAUSS-LEGENDRE QUADRATURE

We next consider integration with respect to the simplest weight function on [-1, 1], namely $\omega(x) \equiv 1$. In this case the resulting quadrature formula (2.5) will approximate the integral

$$\int_{-1}^{1} f(x)\,dx \tag{4.1}$$

The corresponding orthonormal polynomials associated with this weight function are the Legendre polynomials. They can be expressed as

$$p_n(x) = \sqrt{\frac{2n+1}{2}}\, P_n(x), \tag{4.2}$$

where

$$P_n(x) = \frac{1}{(2n)!!} \frac{d^n}{dx^n} (x^2-1)^n, \tag{4.3}$$

this last expression being the Rodrigues formula [6, v.1, Ch. 15].

In order to effectively compute the abscissas and weights of the corresponding quadrature formula (2.5), we must utilize the eigenanalysis of part II. This means that we need the recurrence relation (2.2) from which we can construct the Jacobi matrix A in (2.4). Now the recurrence for the polynomials P_n in (4.3) is

$$nP_n(x) = (2n-1)\ xP_{n-1}(x) - (n-1)P_{n-2}(x)$$

[6]. Combining this with the expression for the normalized polynomials p_n in (4.2) yields the desired recurrence relation:

$$p_n(x) = \left(\frac{2n-1}{n}\right)\sqrt{\frac{2n+1}{2n-1}}\ xp_{n-1}(x) - \left(\frac{n-1}{n}\right)\sqrt{\frac{2n+1}{2n-3}}\ p_{n-2}(x). \qquad (4.4)$$

From (4.4) follows the consistency relation (2.3) and from this follows

$$\frac{c_n}{a_n} = \frac{1}{a_{n-1}} = \frac{n-1}{\sqrt{(2n-1)\ (2n-3)}}\ .$$

Since the $\{b_n\}$ of the general recurrence relation (2.2) are zero here, we have all the entries available to construct the desired matrix A.

5.1 Program and Examples

Exhibit 2 gives a FORTRAN program which enables a user to calculate an n^{th} order Gauss-Legendre approximation to an integral of the form

$$\int_a^b f(x)\,dx.$$

```
C  DOUBLE PRECISION PROGRAM TO DO GAUSS-LEGENDRE QUADRATURE
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION WGTS(100), DD(100), E(100), X(100),
     &Y(100), Z(100,100)
      COMMON A,B
      WRITE(6,1)
1     FORMAT(1X,'INPUT LOWER AND UPPER X-LIMITS')
      READ(5,*) A,B
21    WRITE(6,3)
3     FORMAT(/1X,'INPUT ORDER (LE 100) OF GAUSS FORMULA; INPUT N=0 TO ST
     &OP')
      READ(5,*) N
      IF (N .LT. 1) STOP
      CALL TIMES(D1,T1,IU,IT)
      CALL FORM(N,WGTS,DD,E,Z)
      AINT = 0.D0
      DO 10 I=1,N
         AINT = AINT + WGTS(I)*F(DD(I))
10    CONTINUE
      AINT = 5.D-01*(B-A)*AINT
      CALL TIMES(D1,T2,IUU,ITT)
      ETIM = DFLOAT(IUU-IU)*13.D-06
      WRITE(6,15) N,AINT
15    FORMAT(/1X,'G-LEG.(F;',I3,') = ',D12.6)
      WRITE(6,13) ETIM
13    FORMAT(1X,'EXECUTION TIME = ',F8.3,' SECONDS')
      GO TO 21
      END
C
C
      SUBROUTINE FORM(N,WGTS,DD,E,Z)
      IMPLICIT REAL*8(A-H,O-Z)
C  PROGRAM TO GENERATE WEIGHTS AND ABSCISSAE FOR GAUSSIAN QUADRATURE
C
      DIMENSION  WGTS(N), DD(N), E(N), Z(N,N)
      DO 1 I=1,N
1     DD(I) = 0.D0
      DO 2 I=1,N
      DO 3 J=1,N
         Z(I,J) = 0.D0
3     CONTINUE
      Z(I,I) = 1.D0
2     CONTINUE
      E(1) = 0.D0
      DO 4 I=2,N
4     E(I) = (I-1)/DSQRT(DFLOAT(4*I**2-8*I+3))
      CALL EQRT2S(DD,E,N,Z,N,IER)
      DO 10 J=1,N
      ZN = Z(1,J)**2
      DO 12 I=2,N
12    ZN = ZN + Z(I,J)**2
      ZN = DSQRT(ZN)
      WGTS(J) = 2.D0*(Z(1,J)/ZN)**2
10    CONTINUE
      RETURN
      END
C
C
      FUNCTION F(X)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON A,B
      U = 5.D-01*((B-A)*X + B + A)
C   ENTER INTEGRAND NEXT, AS FUNCTION OF U
      F = 1.D+00 - DABS(U)
      RETURN
      END

R; T=0.04/0.33 13:37:43
```

Exhibit 2

There are two subroutines: subroutine FORM calculates the weights (stored in the array WGTS) and the abscissas (stored in DD); the IMSL subroutine EQRT2S is called by FORM and performs the required eigenanalysis on the matrix A. The program is written in double precision because of the added complexity of the eigenroutine.

Table 2 gives the results of using this program to compute the same integrals as given in Table 1. The time column gives the execution time required for the last value reported in each row.

5.2 Comparison with Gauss-Chebyshev Quadrature

Naturally, Tables 1 and 2 invite comparison. Although the evidence is limited we draw the following general conclusions:

a) Because of the artifical weight function introduced in Gauss-Chebyshev formula, its convergence as measured by the order of the formula (and hence the number of function evaluations) is much slower than that of the Gauss-Legendre formula. The latter however requires added calculation to establish the weights and abscissas. Thus we need to decide (in advance!) whether this additional calculation is worthwhile. This depends on the integrand. As the complexity of its evaluation at various points increases, so does the gain in using fewer function evaluations, hence the Gauss-Legendre formula.

TABLE 2

EXAMPLES OF GAUSS-LEGENDRE QUADRATURE

Integral	N = 3	4	5	6	8	10	20	Time
$\int_0^1 u^{3/2} du$	.39981	.39995	.39998	.39999	—	—	—	.006 sec.
$\int_0^3 e^{2u} du$	199.386	201.143	201.213	201.214	—	—	—	.006 sec.
$\int_0^1 u\sqrt{4-u^2}\, du$	.93462	.93462	—	—	—	—	—	.003 sec.
$\int_0^1 \frac{du}{1+u^4}$	.86752	.86696	.86697	.86697	—	—	—	.006 sec.
$\int_0^1 \frac{2\, du}{2+\sin 10\pi u}$	1.02179	1.19781	1.17553	1.15458	1.10004	1.16146	1.15393	.125 sec.
$\int_{-1}^1 (1-\|u\|)\, du$	1.13934	.95747	1.05515	.98102	.98847	.99248	.99804	.124 sec.

b) Also if the integrand is analytic on a neighborhood of the segment [a, b] (as are the second and third integrands in the Tables), then the rapid convergence of Gauss-Legendre argues in its favor. These two examples show time ratios of about 3:1 in favor of Gauss-Legendre.

c) When the integrand is analytic on (a, b) but not on [a, b] (as are the first and fourth integrands in the Tables), the advantage is still with Gauss-Legendre but somewhat more narrowly.

d) When the integrand is badly behaved with respect to polynomial approximation (as are the final two integrands), the Gauss-Chebyshev method becomes much preferred, because of the ease with which its order is increased.

The general error formula (2.6) for Gauss-Legendre quadrature is

$$\int_{-1}^{1} f(x)dx = G_n(f;\ \text{Leg.}) + \frac{2\cdot 4^n\cdot (n!)^4\ f^{(2n)}(\xi)}{((2n)!)^3\ (2n+1)}\ , \tag{4.5}$$

for $|\xi| < 1$ and $f \varepsilon C^{2n}[-1, 1]$, and this too invites comparison with the corresponding formula (3.2) for Gauss-Chebyshev quadrature. Let GCR (resp., GLR) be the coefficient of $f^{(2n)}(\xi)$ in (3.2) (resp., in (4.5)), and consider the ratio GCR/GLR. Making use of Stirling's approximation it is easy to see that

$$\frac{GCR}{GLR} \sim \frac{(2n+1)e^{2n}}{4^n\; n^{2n+1}} \sim 2\left(\frac{e^2}{4n^2}\right)^n ,$$

asymptotically as $n\to\infty$. This shows that eventually (that is, for large n) the Gauss-Chebyshev formula has the smaller error constant, although initially (for $n \le 10$) GCR $\approx$ 2GLR.

5.3 Evaluation of Double Integrals

The availability of subroutine FORM in the program of Exhibit 2 makes it very easy to implement the product Gauss formula of (2.11) for the case $\omega(x) = \omega(y) = 1$, and the rectangle $a\le y\le b$, $c\le x\le d$. Similarly one could implement a product Gauss-Chebyshev rule, although we have not done so for this report, partly from a reluctance to artificially introduce two weight functions, and partly because of the increased number of function evaluations involved in high order product integral formulas. But as before, if too high an order of Gauss-Legendre is required for the desired accuracy, then the advantage in computation time will pass to Gauss-Chebyshev.

There are several alternate methods of constructing quadrature formulas for multiple integrals [10]. Three popular ones are a) choosing the weights and nodes (= points at which the integrand is evaluated) so as to make the resulting formula exactly integrate polynomials of a certain degree or less; b) minimizing the maximum error over a certain class of possible integrands; and c) statistical (Monte Carlo) sampling.

We looked at several methods of type a), as their theory is the simplest (of the three general methods), and closest in spirit to Gaussian quadrature with its greatest success for integrands having good polynomial approximation properties. Procedures for constructing quadrature rules of the form

$$\int_R f(u)\,du = \sum_{i=1}^{N} \omega_i f(P_i) \tag{4.6}$$

which are exact for all polynomials of degree $\leq d$, and for which N is a minimum are quite involved, and in fact have only been carried out in a few special cases [10]. Particularly interesting from the viewpoints of accuracy and simplicity are formulas due to Radon [10, § 3.12] and Albrecht-Collatz [10, § 8.2]. These are 7 point (N=7 in (4.6)) formulas of degree 5 for the unit square $-1 \leq x,\ y \leq 1$. That is, they will integrate any quintic polynomial in (x, y) exactly over this square, and further, no formula of type (4.6) with N<7 can do this.

The Albrecht-Collatz formula is

$$\int_{-1}^{1}\int_{-1}^{1} f(x, y)\,dx\,dy \approx 4\Big[\tfrac{2}{7}f(0, 0) + \tfrac{25}{168}(f(r, r) +$$

$$f(-r, -r)) + \tfrac{5}{48}(f(s, -t) + f(-s, t) + f(t, -s) + f(-t, s))\Big],$$

where $r^2 = 7/15$, $s^2 = (7+\sqrt{24})/15$, $t^2 = (7-\sqrt{24})/15$.

In Table 3 we present results from using the product Gauss-Legendre and the Albrecht-Collatz formulas on a few double integrals. As expected, the convergence is rapid for analytic integrands, and the Albrecht-Collatz formula usually gives an accuracy of $\pm$ .05% for such integrands, although there is no practical way to predict its accuracy *ex ante*. The fourth integral exhibits quite slow convergence due to the pole at (1, 1). The fifth integral is typical of the sort appearing in optical detection theory. It represents the output of a rectangular detector; the integrand is the irradiance function, J_1 is the Bessel function of first order, and ε is the obscuration factor [4].

TABLE 3

EXAMPLES OF TWO-DIMENSIONAL GAUSS-LEGENDRE QUADRATURE

Integral	N = 3	4	5	10	20	50	A-C	True
$\int_0^{\frac{\pi}{2}}\int_0^{\frac{\pi}{2}} \sin(x+y)\,dxdy$	2.00003	1.99999	1.99999	—	—	—	2.00026	2.00000
$\int_{-1}^{1}\int_{-1}^{1} \cosh(x+y)\,dxdy$	5.52408	5.52439	5.52439	—	—	—	5.52227	5.52439
$\int_0^{2\pi}\int_0^{1} r\sqrt{4-r^2}\,drd\theta$	5.87241	5.87236	5.87236	—	—	—	5.87238	5.87236
$\int_0^{1}\int_0^{1} \frac{dxdy}{1-xy}$	1.58123	1.60599	1.61873	1.63769	1.64303	1.64462	1.55591	1.64493
$\int_{-1.5}^{1.5}\int_{2.5}^{3.5}\left(\frac{J_1(r)-\varepsilon J_1(\varepsilon r)}{r}\right)^2 dxdy$ $r^2 = x^2 + y^2$ $\varepsilon = .5$	.019912	.019728	.019733	—	—	—	.019671	.019733
$\int_0^{1}\int_0^{1}\sqrt{\lvert x-y\rvert}\,dxdy$	.44314	.47133	.48779	.51605	.52697	.53155	.33136	.53333

VI. GAUSS-LAGUERRE QUADRATURE

In this final section we consider integration over the half-line $[a, \infty)$ with the respect to the weight function $\omega(x; \alpha) = x^{\alpha} e^{-x}$. The constraint $\alpha > -1$ is enforced as otherwise $\omega(\cdot; \alpha)$ is not integrable over $[a, \infty)$.

6.1 Special Features

There are two new features in the present situation: the infinite extent of the region of integration, and the parameter α. As already observed in paragraph 2.4, the first feature creates difficulties in establishing the convergence

$$\lim_{n \to \infty} G_n(f; \omega(\cdot; \alpha)) = \int_a^{\infty} f(x)\omega(x; \alpha)dx,$$

but these difficulties are of a theoretical nature and, in any event, have been resolved, as noted earlier.

The use of the free parameter α is of greater practical interest. We have not explicitly encountered its analog before, although one is present. Namely, the Chebyshev and Lengendre polynomials, already used, are orthogonal over $[-1,1]$ with respect to the weight functions $(1-x^2)^{\frac{1}{2}}$ and 1, respectively. Hence they are special cases of polynomials orthogonal over $[-1, 1]$ with respect to the weight function $(1-x^2)^{\beta}$, $\beta > -1$. Any such set of polynomials, is called a set of ultraspherical polynomials, and in particular obeys a recurrence relation of the form (2.2), from which a corresponding Gaussian quadrature formula could be developed as has already been done for the special cases $\beta=-\frac{1}{2}$ and $\beta=0$. The only practical effect of doing so is to slightly shift the corresponding abscissas inside the interval [-1, 1]. (See [9, p. 121] for the pertinent inequalities relating these abscissas to those of the Chebyshev polynomials of the first and second kinds. These abscissas are always symmetric (with respect to 0) for the ultraspherical polynomials.) Unless the weight function $(1-x^2)^\beta$ is explicitly present in an integrand, there seems little point to introducing it artificially (as emphasized earlier, the case $\beta=-\frac{1}{2}$ presents a striking exception to this advice).

A discussion of the zeros of the n^{th} generalized Laguerre polynomial $L_n^{(\alpha)}$ occurs in [9, § 6.31]. In fact, if $x_k^{(n)}$ is the k^{th} zero of $L_n^{(\alpha)}$ then the following bounds are known:

$$\frac{(j_k/2)^2}{n + (\alpha + 1)/2} < x_k^{(n)} <$$

$$(k+(\alpha+1)/2) \cdot \frac{2k+\alpha+1+((2k+\alpha+1)^2+\frac{1}{4}-\alpha^2)^{\frac{1}{2}}}{n+(\alpha+1)/2} \quad ,$$

where $\{j_k\}$ is the sequence of positive zeros of the Bessel function J_α. As is also known [9, § 6.21], $x_k^{(n)}$ is an increasing function of α.

This last property of $x_k^{(n)}$ is of practical importance for Gauss-Laguerre quadrature. For a fixed order n the location of the abscissas can be shifted towards (or away from) the left-hand end point by letting α decrease (resp., increase). In particular the location of the abscissas can be chosen to reasonably coincide with the range of greatest variation of the integrand.

To illustrate this behavior of abscissas (and weights) of Gauss-Laguerre quadrature rules, we display in Table 4 the abscissas and weights for several different 8 point formulas. This table shows how the abscissas drift off to the right as α increases, and also how the corresponding integrand values are given higher weight. The right hand column gives the theoretical sum of the weights, computed from the formula

$$\sum_{k=1}^{n} \omega_k^{(n;\alpha)} = \int_0^\infty x^\alpha e^{-x} dx = \Gamma(\alpha+1).$$

In all cases the actual sum of weights agrees with the theoretical sum to within 1 or 2 units in the 6^{th} decimal place. We can see the sum of the weights first decreasing to a minimum (actual value = 0.885603 when α = 0.461632), and then increasing without bound. This information follows from standard properties of the gamma function [13, Ch. 6].

TABLE 4

GAUSS-LAGUERRE ABSCISSAS AND WEIGHTS

		k = 1	2	3	4	5	6	7	8	Weight Sum
α=-.75	abs.	0.034478	0.567861	1.733810	3.580823	6.200283	9.758005	14.584774	21.539966	
	wgt.	2.693882	0.731633	0.17492	0.023683	0.001576	0.000043	0.000000	0.000000	3.625608
α=-.5	abs.	0.074792	0.677249	1.905114	3.809476	6.483145	10.093324	14.972627	21.984273	
	wgt.	1.015859	0.561295	0.167620	0.025761	0.001865	10.000054	0.000000	0.000000	1.772454
α=-.25	abs.	0.120233	0.789215	2.077536	4.038084	6.764989	10.426788	15.357881	22.425274	
	wgt.	0.557369	0.468574	0.168247	0.028898	0.002258	0.000070	0.000000	0.000000	1.225417
α=0.	abs.	0.170280	0.903702	2.251087	4.266700	7.045905	10.758516	15.740679	22.063132	
	wgt.	0.369189	0.418787	0.175795	0.033343	0.002795	0.000091	0.000001	0.000000	1.
α=.5	abs.	0.282634	1.139874	2.601525	4.724115	7.605256	11.417182	16.499411	23.730004	
	wgt.	0.227139	0.393595	0.212909	0.047877	0.004543	0.000162	0.000002	0.000000	.886227
α=1.	abs.	0.409384	1.384963	2.956255	5.181943	8.161710	12.070055	17.249736	24.585955	
	wgt.	0.187633	0.438985	0.289996	0.075141	0.007933	0.000309	0.000003	0.000000	1.
α=2.	abs.	0.699330	1.898816	3.677615	6.099295	9.267426	13.360738	18.728139	26.268641	
	wgt.	0.224798	0.799531	0.713671	0.231541	0.029136	0.001308	0.000016	0.000000	2.
α=3.	abs.	1.029962	2.439914	4.413187	7.019210	10.365359	14.634328	20.180847	27.917193	
	wgt.	0.447659	2.129575	2.370081	0.913728	0.132197	0.006668	0.000090	0.000000	6.

6.2 Program and Examples

Table 4 was derived from the FORTRAN program in Exhibit 3. This program enables a user to compute an approximation to the integral

$$\int_T^{\infty} f(x)\,dx \ ;$$

the user must supply as input a value of the parameter α, the order N of the corresponding Gauss-Laguerre formula, and the value T of the lower endpoint. As in the program of Exhibit 2 for Gauss-Legendre quadrature, there are two subroutines: FORM and EQRT2S (from IMSL), which together effect the computation of the relevant weights and abscissas.

Table 5 displays a few examples of Gauss-Laguerre quadrature. The first integrand is a nice entire function for which the choice $\alpha = 0$ leads to rapid convergence. The second integrand exhibits slowly decaying oscillatory behavior and convergence is poor. Probably $\alpha = 0$ would be the default choice here too, although the integrand is inherently badly behaved for quadrature. The next integrand has a singularity at $x = 0$; the feature in general would suggest a value of $\alpha < 0$, and the factor $x^{-\frac{1}{2}}$ in the integrand in turn leads to $\alpha = -.5$ as the preferred choice. The last integrand is (up to a constant factor) the type occuring in integration of

```
C  PROGRAM TO DO DOUBLE PRECISION GENERALIZED GAUSS-
C  LAGUERRE QUADRATURE
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION  WGTS(100), D(100), E(100), Z(100,100)
      COMMON AL
50    WRITE(6,1)
1     FORMAT(/1X,'INPUT ALPHA AND N')
      READ(5,*) AL,N
      WRITE(6,4)
4     FORMAT(1X,' PRINT WEIGHTS AND ABSCISSAE? INPUT 0(NO) OR 1(YES)')
      READ(5,*) KG
      CALL FORM(AL,N,WGTS,D,E,Z,KG)
      WRITE(6,3)
3     FORMAT(/1X,'THIS PROGRAM WILL NOW ESTIMATE THE INTEGRAL OF F FROM
     & T TO INFINITY; INPUT T')
      READ(5,*) T
      QNF = 0.
      DO 15 I=1,N
15    QNF = QNF + WGTS(I)*F(T+D(I))*(1.+T/D(I))**AL
      QNF = QNF*DEXP(-T)
      WRITE(6,12) N, QNF
12    FORMAT(/1X,'G-L QUAD(F;',I3,') = ',D12.6)
      WRITE(6,2)
2     FORMAT(/1X,'RESTART?  INPUT 0(NO)  OR  1(YES)')
      READ(5,*) NR
      IF (NR .NE. 1)  STOP
      GO TO 50
      END
C
C
      SUBROUTINE FORM(AL,N,WGTS,D,E,Z,KG)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION  WGTS(N), D(N), E(N), Z(N,N)
      DO 1 I=1,N
1     D(I) = 2.D0*DFLOAT(I)+AL-1.D0
      DO 2 I=1,N
      DO 3 J=1,N
         Z(I,J) = 0.D0
3     CONTINUE
      Z(I,I) = 1.D0
2     CONTINUE
      E(1) = 0.D0
      DO 4 I=2,N
4     E(I) = -DSQRT(DFLOAT(I-1)*(I-1+AL))
      CALL EQRT2S(D,E,N,Z,N,IER)
      IF (KG .EQ. 0) GO TO 20
      WRITE(6,5) (D(I),I=1,N)
5     FORMAT(/1X,'ABSCISSAE = ',/,5(10F12.6,/))
20    DO 10 J=1,N
      ZN = Z(1,J)**2
      DO 12 I=2,N
12    ZN = ZN + Z(I,J)**2
      ZN = DSQRT(ZN)
      WGTS(J) = (Z(1,J)/ZN)**2
      WGTS(J) = DGAMMA(AL+1.)*WGTS(J)
10    CONTINUE
      IF(KG .EQ. 0) RETURN
      WRITE(6,15) (WGTS(J),J=1,N)
15    FORMAT(/1X,'WEIGHTS = ',/,5(10F12.6,/))
      RETURN
      END
C
C
C
C
C
C
C
C
C
C
C
C
C
C
      FUNCTION F(X)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON AL
C *** DEFINE INTEGRAND G NEXT
      Z = 1./X
      G = (1.-DEXP(-X)-DEXP(-Z))*Z
      F = G*(X**(-AL))*DEXP(X)
      RETURN
      END
EOF:
```

Exhibit 3

TABLE 5

EXAMPLES OF GAUSS-LAGUERRE QUADRATURE

Integral	α	N = 3	4	5	6	8	10	15	True
$\int_0^\infty e^{-2x}\cosh x dx$	-.5	.758401	.731909	.716048	.706168	.694937	.688758	.681004	
	0	.656212	.663656	.665826	.666437	.666650	.666666	.6666667	.666667
	1	.423476	.468522	.500499	.523943	.555565	.575758	.604167	
$\int_0^\infty \frac{\cos x dx}{1+x^2}$	-.9	.644090	.515595	.658017	.559423	.561821	.563917	.596039	
	-.5	.720825	.511405	.670778	.544987	.559617	.568563	.602658	.577864
	0	.686725	.525229	.623518	.529730	.547787	.561743	.586817	
	1	.249619	.428776	.379850	.476303	.497871	.509270	.508757	
$\int_0^\infty \frac{e^{-2x}dx}{x}$	-.9	2.40177	2.22545	2.11203	2.03118	1.92088	1.84730	1.73506	
	-.5	1.25106	1.25306	1.25329	1.25331	1.25331	———	———	1.25331
	0	.746209	.816623	.863535	.897797	.945607	.978133	1.02863	
$\int_2^\infty \frac{x^3 dx}{e^x-1}$	0	5.31728	5.31751	5.31759	5.31760	5.31760	———	———	
	1.5	.478276	4.88794	4.95843	5.00901	5.07680	5.12015	5.18140	5.31760
	3	.391210	4.17133	4.34986	4.48029	4.65813	4.77370	4.93945	

Planck's equation for radiant graybody sterance. The interval of integration $[2,\infty)$ corresponds roughly to the wavelength band $(0, 7194]$. Surprisingly enough here, the "natural" choice $\alpha = 3$ is considerably less effective than smaller α's. The reason for this can be deduced from Table 4; since the integrand $x^3/(e^x-1)$ is rapidly decreasing after its peak at $x \approx 2.8$, it is advantageous to have the abscissas clustered closer to the left end point ($= 2$, in our example), and as we know, this requires smaller values of α.

VII. FINAL EXAMPLES AND SUMMARY

In this report we have advanced a fast and efficient method for carrying out numerical integration by means of Gaussian quadrature. We have stressed that Gaussian methods should only be applied in situation where the integrand has the property of good polynomial approximation. In the contrary cases, when either the integrand is insufficiently differentiable or has a singularity on or near the boundary of the region of integation, other methods should be adopted. In particular, in the first case some version of the trapazoid rule, such as Romberg integration, might be tried (see Introduction). On the other hand, the treatment of singularities is often a matter of *ad hoc* techniques, several of which are suggested in [14].

Sometimes a simple change of variable can greatly expedite the quadrature process. We give next two final examples, both of which can be viewed either as integrands with singularity at one end point of a finite interval or as integrands analytic over an infinite interval. In the first case the change of variables does not help at all, while in the second case the improvement is dramatic.

C

Example 1

$$\int_0^1 (1-e^{-x}-e^{-\frac{1}{x}})\frac{dx}{x} = \int_1^\infty (1-e^{-x}-e^{-\frac{1}{x}})\frac{dx}{x} = \gamma = .577216,$$

where γ is Euler's constant. The results of three attempts at integration by our methods are given next.

Gauss-Chebyshev

N=	10	25	50	75	100	150	200
Value	.579836	.577631	.577316	.577257	.577235	.577221	.577214 (time=.024 sec.)

Gauss-Legendre

N=	5	6	7	8	9	10	11	12	15
Value	.577684	.577450	.577155	.577165	.577218	.5772277	.577218	.577214	.577216 (time=.055 sec.)

Gauss-Laguerre

N=	5	6	7	8	10	12	15	20
Value								
α = -.9	.52544	———	———	———	.55260	———	.56126	.56545
-.75	.52999	.53823	———	.54848	.55456	.55855	.56249	.56635
-.5	.53134	.53923	.54485	.54907	.55494	.55470	.56267	.56646
-.25	.52840	———	———	———	.55326	———	.56149	.56555
0.	.52257	.53168	———	———	.55009	———	.55931	.56389

We can see from these results that conversion from the interval (0,1] to [1,∞) has not achieved any worthwhile results; the Gauss-Laguerre formulas are all converging very slowly. The Gauss-Chebyshev method has essentially converged by N = 200; the error in the 6^{th} decimal place is due to the inaccuracy of the single precision arithmetic.

Example 2

$$\int_0^1 (\log x)^n dx = (-1)^n \int_0^\infty y^n e^{-y} dy = (-1)^n n!$$

In this example we see that the change of variable converts an intractable integral over (0,1) into a very simple integral over [0,∞) which can either be evaluated in closed form (using integration by parts), or integrated very quickly and accurately by the Gauss-Laguerre method (using either $\alpha=0$ or $\alpha=n$). By contrast, observe the result of attacking the logarithmic integral directly in the case n=4.

Gauss-Chebyshev

N=	10	25	50	100	150	200	300	500
Value	23.6216	24.4664	24.3403	24.1803	24.1153	24.0819	24.0490	24.0245 (time=.039 sec.)

Gauss-Legendre

N=	10	15	20	25	30	40	50	75	90
Value	17.4324	19.7869	21.0005	21.7232	22.1952	22.7634	23.0857	23.4809	23.6001 (time=7.45 sec.)

In conclusion, if asked to recommend a single all-purpose integration routine, our choice would have to be the Gauss-Chebyshev formula (even for infinite intervals, by truncation). Its simplicity and the speed with which its order can be increased are the decisive factors.

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REFERENCES

1. P. Davis and P. Rabinowitz, Methods of Numerical Integration, (Academic Press, New York, 1975).

2. H. Wilf, Mathematics for the Physical Sciences, (Wiley, New York, 1962).

3. G. Golub and J. Welsch, "Calculation of Gauss Quadrature Rules", Math. Comp. 23 221-230, (1969).

4. K. Seyrafi, Electro-Optical Systems Analysis, Electro-Optical Research Co., Los Angeles, CA (1973).

5. G. Freud, Orthogonal Polynomials, (Pergamon Press, Oxford, England, 1971).

6. I. Natanson, Constructive Function Theory, Vols. 1 and 2, United States Atomic Energy Commission Translation Series, 1961. published by Ungar, New York, 1964.

7. A. Stroud and D. Secrest, Gaussian Quadrature Formulas (Prentice-Hall, Englewood Cliffs, NJ 1966).

8. B. Von Sydow, "Error estimates for Gaussian quadrature formulas", Numer. Math. 29, 59-64, (1977/78).

9. G. Szego, Orthogonal Polynomials (Amer. Math Society, Providence, RI 1959).

10. A. Stroud, Approximate Calculation of Multiple Integrals (Prentice-Hall, Englewood Cliffs, NJ 1971).

11. P. Rabinowitz and G. Weiss, "Tables of abscissas and weights for numerical evaluation of integrals of the form $\int_0^\infty e^{-x}x^n f(x)dx$", Math. Tables and Other Aids to Computation 13, 285-293, (1959).

12. A. Ghizzetti and A. Ossicini, Quadrature Formulae, (Academic Press, New York, 1970).

13. M. Abramowitz and I. Stegun, Eds. Handbook of Mathematical Functions (National Bureau of Standards, Washington, DC 1964).

14. F. Acton, Numerical Methods that Work (Harper and Row, New York, 1970).

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A method for accurate numerical integration is proposed and illustrated by a variety of examples. The method depends on an ability to efficiently evaluate the weights and abscissas of Gaussian quadrature formulas, and software to achieve this purpose is also presented.

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